

Dimethyl ethylmalonate  
26717-67-9 | DTXSID70181214

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.39e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.39e-01

Confidence level: 8.72e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,2-Phenylenediamine</div> <div>Measured: 4.14e-01</div> <div>Predicted: 8.53e-04</div>	<div>Image not found</div> <div>1,3-Diethenylbenzene</div> <div>Measured: 9.00e-01</div> <div>Predicted: 8.63e-01</div>	<div>Image not found</div> <div>4-Bromophenol</div> <div>Measured: 4.10e-01</div> <div>Predicted: 2.33e-02</div>
<div>Image not found</div> <div>Acetic acid, chloro-, 1-methylethyl ester</div> <div>Measured: 2.69e-01</div> <div>Predicted: 6.23</div>	<div>Image not found</div> <div>Benzene, (iodomethyl)-</div> <div>Measured: 3.00e-01</div> <div>Predicted: 1.97e-01</div>	